I INTRODUCTION

Developing Advanced Combustion Engine Technologies

On behalf of the Department of Energy's Office of FreedomCAR and Vehicle Technologies, we are pleased to introduce the Fiscal Year (FY) 2005 Annual Progress Report for the Advanced Combustion Engine R&D Sub-Program. Advanced internal combustion engines are a key element in the pathway to achieving the goals of the President's FreedomCAR and Hydrogen Fuel Initiative for transportation. The mission of the FreedomCAR and Vehicle Technologies (FCVT) Program is to develop more energy-efficient and environmentally friendly highway transportation technologies that enable America to use less petroleum. The Advanced Combustion Engine R&D Sub-Program supports this mission and the President's initiatives by removing the critical technical barriers to commercialization of advanced internal combustion engines for light-, medium-, and heavy-duty highway vehicles that meet future Federal and state emissions regulations. The primary objective of the Advanced Combustion Engine R&D Sub-Program is to improve the brake thermal efficiency of internal combustion engines from

- 30 to 45 percent for light-duty applications by 2010
- 40 to 55 percent for heavy-duty applications by 2013

while meeting cost, durability, and emissions constraints. R&D activities include work on combustion technologies that increase efficiency and minimize in-cylinder formation of emissions, as well as aftertreatment technologies that further reduce exhaust emissions. Research is also being conducted on approaches to produce useful work from waste engine heat through the development and application of thermoelectrics, turbochargers that include electricity generating capability, and incorporation of energy-extracting turbines.

Another research area is on highly efficient and low-emission hydrogen-fueled internal combustion engines, providing an energy-efficient interim hydrogen-based powertrain technology in the ultimate transition to hydrogen fuel cell powered transportation vehicles. This R&D promotes the longer-term FreedomCAR Partnership goal to help the nation reduce both energy use and greenhouse gas emissions, thus improving energy security by dramatically reducing dependence on petroleum for transportation. Hydrogen engine technologies being developed have the potential to provide diesel-like engine efficiencies with near-zero air pollution and greenhouse gas emissions.

This introduction serves to outline the nature, current progress, and future directions of the Advanced Combustion Engine R&D Sub-Program. The research activities of this Sub-Program are planned in conjunction with the FreedomCAR and Fuel Partnership, and the 21st Century Truck Partnership, and are carried out in collaboration with industry, national laboratories, and universities. Because of the importance of clean fuels in achieving low emissions, R&D activities are closely coordinated with the relevant activities of the Fuel Technologies Sub-Program, also within the Office of FreedomCAR and Vehicle Technologies.

Background

The compression ignition direct injection (CIDI) engine, an advanced version of the commonly known diesel engine, is a promising advanced combustion engine technology for achieving dramatic energy efficiency improvements in light- and heavy-duty vehicles. Light-duty vehicles with CIDI engines can compete directly with gasoline engine hybrid vehicles in terms of fuel economy and consumer-friendly driving characteristics. Light-duty hybrid vehicles using CIDI engines are projected to have energy efficiencies that are competitive with hydrogen fuel cell vehicles. The primary hurdles that must be overcome to realize increased use of CIDI engines in light-duty vehicles are the higher cost of these engines compared to conventional gasoline engines and compliance with the U.S. Environmental Protection Agency's (EPA's) Tier 2 regulations which are phasing-in from 2004-2009. The Tier 2 regulations require all light-duty vehicles to meet the same emissions standards, regardless of the powertrain. This requirement can be achieved through the addition of catalytic emission control technologies, though these technologies are much less mature and are severely affected by fuel sulfur, unlike gasoline engine catalysts. Even the reduction of diesel fuel sulfur content to below 15 ppm starting in June 2006 (retailers will be allowed to sell diesel fuel having up to 22 ppm sulfur through October 15 as part of the transition) does not assure that CIDI engine catalytic emission control devices will be durable and cost-effective. A great need still exists to reduce the emissions produced from CIDI engines without degrading their already excellent efficiency, which also has the potential for further gains.

The CIDI engine is already the primary engine for heavy-duty vehicles because of its high efficiency and outstanding durability. However, the implementation of more stringent heavy-duty engine emission standards, which are to be phased in starting in 2007 (100% implementation in 2010), is predicted to cause a reduction in fuel efficiency due to the exhaust emission control devices needed to meet both the oxides of nitrogen (NOx) and particulate matter (PM) emissions regulations.

Given these challenges, the Advanced Combustion Engine Technologies Sub-Program is working toward achieving the following objectives:

- Research and develop advanced combustion regimes to enable high-efficiency engines with near-zero emissions. These advances (or this understanding) will reduce the size and complexity of emission control devices and minimize any impact these devices have on vehicle fuel efficiency.
- Increase overall engine efficiency through fundamental improvements such as advanced combustion processes, reduction of parasitic losses, and energy recovery from waste heat.
- Improve the effectiveness and efficiency of emission control devices to enable advanced combustion engines to achieve significant penetration in the light-duty market and maintain their application in heavy-duty vehicles.
- Develop highly efficient hydrogen engine technologies with near-zero air pollution and greenhouse gas emissions.

Technology Status

Recent advances in fuel injection systems have made the CIDI engine very attractive for light-duty vehicle use by taming combustion noise, and the public is discovering that diesel engines offer outstanding driveability and fuel economy. The change-over to ultra-low sulfur diesel fuel should remove the offensive odors associated with diesel engines and further improve their prospects for wider use in light-duty vehicles. Mercedes-Benz has recently confirmed that it will introduce five diesel models in the U.S. beginning in fall 2006. Honda, BMW, Nissan and the Chrysler group each have confirmed plans to add diesels to their lineups over the next three to four years. In heavy-duty vehicles, the CIDI engine remains the engine of choice because of its high efficiency and durability. While both light- and heavy-duty CIDI engines continue to become more reliable, quiet, and efficient, they require development of emission control technology to meet future emission regulations.

The technology for controlling PM emissions from CIDI engines (particulate traps) is highly effective and is entering commercial markets in applications (mostly transit buses) where duty cycles and engine strategies create adequately high exhaust temperatures to ensure regeneration, and where ultra-low-sulfur fuel is available. Cost, energy penalty due to back-pressure, and durability are likely to be the important characteristics for choosing which PM control technology to employ for a given application, though the type of NOx control device used will also play a role in specifying a PM trap and where it will be placed.

Technology for control of NOx is not nearly as mature as the technology for control of PM. Competing technologies include lean NOx traps (LNTs) and selective catalytic reduction (SCR) employing urea or hydrocarbons (from the onboard diesel fuel) for regeneration. Of these technologies, SCR using urea as a reductant is the current leader in terms of having the lowest fuel penalty and highest durability (SCR using hydrocarbons has lower conversion efficiency).

Development of LNTs, also known as NOx adsorbers, has shown rapid improvement. NOx adsorbers appear to be able to achieve the Tier 2 Bin 5 light-duty vehicle emission levels when new using ultra-low sulfur fuel, although full-useful vehicle life emissions have not yet been demonstrated. NOx adsorbers for heavy-duty vehicles are less well-developed based on the size of these units compared with engine displacement (being over twice as large as those required for light-duty vehicles). The "not-to-exceed" operating conditions, typically generating high exhaust temperatures, are further problematic for LNTs. The durability of NOx adsorbers is still in question since they are sensitive to even small amounts of sulfur in the fuel or engine lubricant (urea-SCR catalysts are less sensitive to sulfur). The other major concern about NOx adsorbers is their effect on fuel consumption and cost. NOx adsorbers use fuel to regenerate instead of urea, and current fuel “penalties” for regeneration are declining but still in the range of five to ten percent of total fuel flow.

Current Sub-Program Focus

An optimum solution to CIDI engine emissions is to alter the combustion process in ways that produce emissions at levels that don’t need ancillary devices for emissions control, or greatly reduce the requirements of these systems, yet maintain or increase the engine efficiency. This is the concept behind new combustion regimes such as homogeneous charge compression ignition (HCCI) and other modes of low-temperature combustion (LTC), which result in greatly reduced levels of NOx and PM emissions (emissions of hydrocarbons and carbon monoxide still exist and must also be controlled). Significant progress is being made in these types of combustion systems, and performance has been demonstrated over increasingly larger portions of the engine speed/load map. The major issues of this R&D include fuel mixing, control of air intake flow and its temperature, control of combustion initiation, and application over a wider portion of the engine operating range. Control of fuel injection and valve opening independent of piston movement appear to be highly desirable for HCCI and LTC engines. Fuel composition is another important variable for these engines, and techniques are being explored to exploit fuel properties advantageously to help control combustion and lower emissions.

Complex and precise engine and emission controls will require sophisticated feedback systems employing new types of sensors. NOx and PM sensors are in the early stages of development and require additional advances to be cost-effective and reliable, but are essential to control systems for these advanced engine/aftertreatment systems. Much progress has been made, but durability and cost remain as the primary issues with these sensors.

Advanced fuel formulations and fuel quality are also crucial to achieving higher energy efficiencies and meeting emissions targets. The EPA rule mandating that the sulfur content of highway diesel fuel be reduced to less than 15 ppm starting in 2006 will greatly benefit the effectiveness, efficiency, and durability of emission control devices. The EPA has reported that based on pre-compliance reports, 95 percent of all the diesel fuel being produced should be less than 15 ppm sulfur by June 2006 (retailers will be allowed to sell diesel fuel having up to 22 ppm sulfur through October 15 as part of the transition). The addition of non-petroleum components such as biodiesel can have beneficial effects on emissions while providing lubricity enhancement to ultra-low-sulfur diesel fuel.

Waste heat recovery is not currently implemented on either light- or heavy-duty CIDI vehicles and represents an area of significant potential for efficiency improvements.

Future Directions

Internal combustion engines have a maximum theoretical fuel conversion efficiency that is similar to that of fuel cells; it approaches 100%. The primary limiting factor to approaching these theoretical limits of conversion efficiency is the high irreversibility in traditional premixed or diffusion flames. Multiple studies agree that combustion irreversibility losses consume more than 20% of the available fuel energy and are a direct result of flame front combustion. Examples of "new combustion regimes" that might lower the irreversibility losses include dilute combustion with low peak temperatures, higher expansion of combustion gases, and increased reactant temperature. The engine hardware changes needed to execute these advanced combustion regimes include variable fuel injection geometries, methods to produce very high manifold pressures, compound compression and expansion cycles, variable compression ratio, and improved sensors and control methods. Recent analyses show that reducing the inherent combustion losses must be coupled with other cycle improvements for full effectiveness.

The other areas where there is large potential for improvements in internal combustion engine efficiency are losses from the exhaust gases and heat transfer losses. Potential ways that these losses might be reduced include compound compression and expansion cycles achieved by valve timing, use of turbine expanders, application of thermoelectric generators, and lean-burn and stratified-charge engines.

Fuels can also play an important role in reducing combustion irreversibility losses. Preliminary analyses show that combustion irreversibility losses per mole of fuel are considerably less for hydrogen than for hydrocarbon fuels. This finding is consistent with the understanding that combustion irreversibility losses are reduced when combustion is occurring nearer equilibrium (high temperature), since hydrogen has the highest adiabatic flame temperature of the fuels studied to date. This bodes well for the development of highly efficient hydrogen-fueled internal combustion engines.

Goals and Challenges

The Advanced Combustion Engine R&D Sub-Program has five activities:

- Combustion and Emission Control R&D
- Light Truck Engine R&D (completed)
- Heavy Truck Engine R&D
- Waste Heat Recovery
- Health Impacts

<u>Combustion and Emission Control R&D</u>

The Combustion and Emission Control R&D activity focuses on enabling technologies for energy-efficient, clean vehicles powered by advanced internal combustion engines (ICEs) using clean hydrocarbon-based and non-petroleum-based fuels and hydrogen. R&D has been focused on developing technologies for light-, medium-, and heavy-duty CIDI engines and is being transitioned to developing technologies for advanced engines operating in combustion regimes that will further increase efficiency and reduce emissions to near-zero levels.

Fuel efficiency improvement is the overarching focus of this activity, but resolving the interdependent emissions challenges is a critical first step. (Penetration of even current-technology CIDI engines into the light-duty truck market would reduce fuel use by 30-40% compared to a gasoline vehicle.) The major challenges facing CIDI emission control systems across all three platforms are similar: durability, cost, and fuel penalty (or in the case of urea-SCR, urea infrastructure development). Full-life durability has yet to be demonstrated for either light- or heavy-duty systems. Nor have these systems demonstrated the ability to "bounce back" following exposure to fuel sulfur levels higher than 15 ppm, which could occur periodically due to cross-contamination of fuels and outright fuel substitution mistakes.

The FreedomCAR and Fuel Partnership goals for internal combustion engines (ICEs) are as follows:

- By 2010, an ICE powertrain system costing $30/kW, having a peak brake engine efficiency of 45% and meeting applicable emission standards.
- An ICE powertrain system operating on hydrogen with a cost target of $45/kW by 2010 and $30/kW in 2015, having a peak brake thermal efficiency of 45% and meeting applicable emission standards.

The following goals are energy-efficiency improvement targets for advanced combustion engines suitable for passenger cars and light trucks; they also address technology barriers and R&D needs that are common between light- and heavy-duty vehicle applications of advanced combustion engines.

- By 2007, achieve peak CIDI engine efficiency of at least 42% and, combining the advanced engine with emission control devices, meet EPA Tier 2, Bin 5 requirements in a light-duty vehicle using diesel fuel (specified by the Fuels Technology sub-program) with a fuel efficiency penalty of not more than 2%.
- By 2010, develop the understanding of novel low-temperature engine combustion regimes needed to simultaneously enable peak engine efficiency of 45% and an aftertreatment fuel efficiency penalty of less than 1%.

The targets for passenger cars, derived primarily by the FreedomCAR Partnership, are shown in Table 1. Achieving emissions compliance for CIDI engines in light-duty vehicles will provide a “quantum leap” (~30%) fuel efficiency improvement over port-fuel-injected spark ignition engines. In the longer term, further advancing engine efficiency along with reducing the emission control energy penalty will gain another 15-18% fuel efficiency improvement beyond today’s technology. Longer range goals are set for hydrogen-fueled combustion engines.

<u>Heavy Truck Engine R&D</u>

The long-term (2013) goal of this activity is to develop the technologies that will increase the thermal efficiency of heavy-duty diesel engines to at least 55% while reducing emissions to near-zero levels (see Table 2). More specifically,

- By 2007, increase the peak thermal efficiency of heavy-duty engines to 50% while meeting EPA 2010 emission standards.
- By 2013, increase the peak thermal efficiency of heavy truck engines to 55% while meeting prevailing EPA emission standards.

The interim goal for fiscal year 2005 of achieving 45% efficiency while demonstating 2007 emissions standards was successfully achieved. This activity also supports the goal of 21st Century Truck Partnership to develop and validate a commercially viable, 50% efficient, emissions-compliant engine system for Class 7 and 8 highway trucks by 2010.

Researchers will need to simultaneously increase thermal efficiency of heavy-duty truck engines significantly while lowering emissions. To date, all the 2005 targets have been achieved except for emissions systems durability. By 2007, efficiency will need to be increased further while NOx emissions are reduced by 83 percent. Achieving these technical targets will require sustained R&D activities along several fronts.

Table 1. Technical Targets for the Combustion and Emission Control Activity

Characteristics	Units	Fiscal Year			
		2007	**2009**	**2010**	**2015**
FreedomCAR Goals					
ICE Powertrain					
Peak Brake Thermal Efficiency (HC Fuel) (H_2 Fuel)	%	42	44	45 45	 45
Cost (HC Fuel) (H_2 Fuel)	$/kW			30 45	 30
(H_2-ICE)				30 (2015)	
Reference Peak Brake Thermal Efficiency[a]	%	32	34	35	
Target Peak Brake Thermal Efficiency/Part-Load Brake Thermal Efficiency (2 bar BMEP[b] @1500 rpm)	%	41/27	43/29	45/31	
Powertrain cost[c,d]	$/kW	30	30	30	
Emissions[e]	(g/mile)	Tier 2, Bin 5	Tier 2, Bin 5	Tier 2, Bin 5	
Durability[e]	Hrs.	5,000	5,000	5,000	
Thermal efficiency penalty due to emission control devices[f]	(%)	<2	<1	<1	

[a] Current production, EPA compliant engine

[b] Brake mean effective pressure

[c] High-volume production: 500,000 units per year

[d] Constant out-year cost targets reflect the objective of maintaining powertrain (engine, transmission, and emission control system) system cost while increasing complexity.

[e] Projected full-useful-life emissions for a passenger car/light truck using advanced petroleum-based fuels as measured over the Federal Test Procedure as used for certification in those years.

[f] Energy used in the form of reductants derived from the fuel, electricity for heating and operation of the devices, and other factors such as increased exhaust back-pressure, reduce engine efficiency.

Table 2. Technical Targets for Heavy Truck Diesel Engine R&D

Characteristics	Fiscal Year		
	2005 Status	**2007**	**2013**
Engine thermal eff., %	>45	>50	>55
NO_x emissions, g/bhp-hr	<1.2	<0.20	<0.20
PM emissions[1], g/bhp-hr	<0.01	<0.01	<0.01
Stage of Development	prototype	prototype	prototype
Durability, miles (equivalent)	>200,000 (target)	>400,000	

[1] Using 15-ppm-sulfur diesel fuel

Waste Heat Recovery

Recovery of energy from the engine exhaust represents a potential for 10% or more improvement in overall engine thermal efficiency. Turbochargers are used to recover part of this energy. Turbochargers currently have efficiencies of around 50 to 58%, which could be increased to 72 to 76% with enhancements such as variable geometry. An electrically driven turbocharger with increased transient response would be another approach. Turbocompounding and direct thermal-to-electric conversion could also improve the overall thermal efficiency. Bulk semiconductor thermoelectric devices are currently 6 to 8% efficient. Recent developments in quantum well thermoelectrics suggest a potential improvement to over 20% is possible.

The longer-term goal of this activity is to develop the technologies for recovering engine waste heat and converting it to useful energy that will improve overall diesel engine thermal efficiency to 55% while reducing emissions to near-zero levels. More specifically,

- By 2010, enable commercially viable turbocompound units that can produce more than 10 kW of additional power from light-duty engine waste heat recovery.
- By 2012, enable commercially viable turbocompound units that can produce up to 40 kW of additional power from heavy-duty engine waste heat recovery.
- By 2012, achieve at least 21% efficiency in quantum well thermoelectric devices for waste heat recovery.

This activity also supports the overall engine efficiency goals of the FreedomCAR and Fuel Partnership and 21st Century Truck Partnership.

The technical targets for the waste heat recovery R&D activities are listed in Table 3. Significant progress will be needed to meet the 2008 targets. Ongoing and newly awarded projects are focused on achieving this progress.

Health Impacts

The Health Impacts Research activity supports the FreedomCAR and Vehicle Technologies mission to ensure that the more energy-efficient advanced combustion engine technologies are environmentally friendly

Table 3. Technical Targets for Waste Heat Recovery

Characteristics	**Units**	**2005 Status**	**2008**
Electrical turbocompound system			
Class 7-8 trucks			
Fuel economy improvement	%	<5	>10
Power	kW	>40	>30
Projected component Life	Hrs.	<10	>10,000
Thermoelectric Devices			
Efficiency bulk semiconductor quantum well	%	6-8 14	-- >15
Projected cost/output (250,000 production volume)	$/kW	TBD	180

and do not produce adverse health impacts. This activity seeks to identify, analyze, quantify, and, if possible, avoid potentially deleterious health impacts of new vehicle technologies, specifically of emissions from vehicles using conventional as well as alternative fuels. The emphasis is to place transportation emissions in a proper context, focusing on providing a balance to the portfolio of health research conducted by others.

The goal of the Health Impacts Research activity is to provide a sound scientific basis for the relationship between mobile-source emissions from new vehicle technologies (engines, fuels, aftertreatment, and engine operating conditions or vehicle drive cycles) and their health impacts; more specifically, it is to identify and quantify potential health hazards associated with the use of fuels in transportation vehicle engines.

Project Highlights

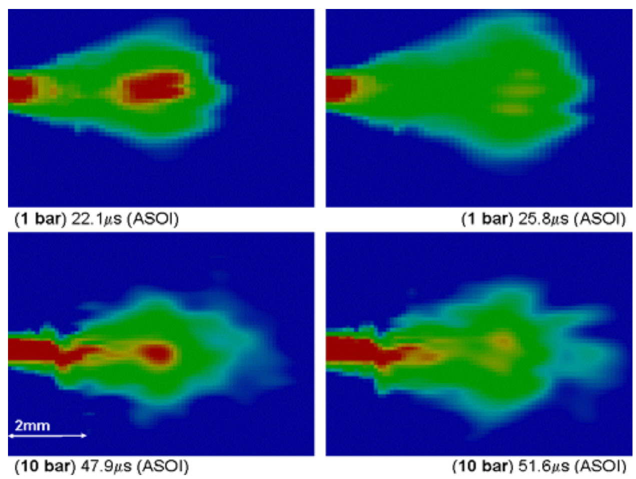
The following projects highlight progress made in the Advanced Combustion Engine R&D Sub-Program during FY 2005.

Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

The objective of these projects is to identify how to achieve more efficient combustion with reduced emissions from advanced technology engines.

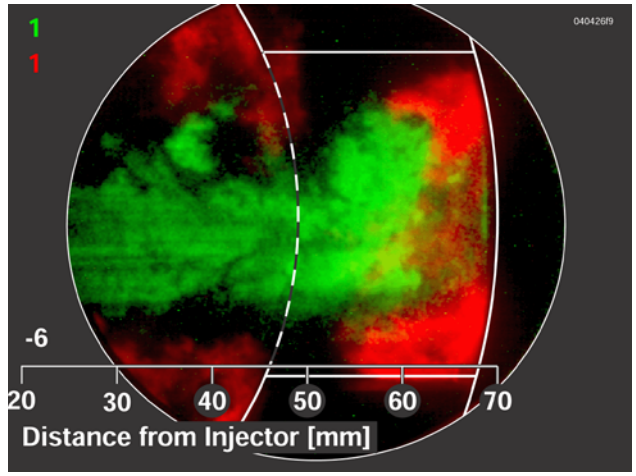
- Using X-rays from their Advanced Photon Source, Argonne National Laboratory (ANL) completed the first-ever phase-contrast images of fuel sprays, which revealed the cavitation and ligaments in a spray as it emerges from the nozzle.
- Sandia National Laboratories (SNL) identified "under-mixed" fuel as a dominant source of CO emissions (and combustion inefficiency) for high-dilution operating conditions, and clarified the relative importance of complete combustion, heat transfer, and combustion phasing on the fuel conversion efficiency of low-temperature combustion regimes.
- SNL studied spray, combustion, and pollutant formation for a typical early-injection, LTC operating condition using multiple, simultaneous imaging diagnostics which provided new understanding of in-cylinder processes.



ANL X-ray Images of Fuel Injector Spray at 1 Bar and 10 Bar Ambient Pressure

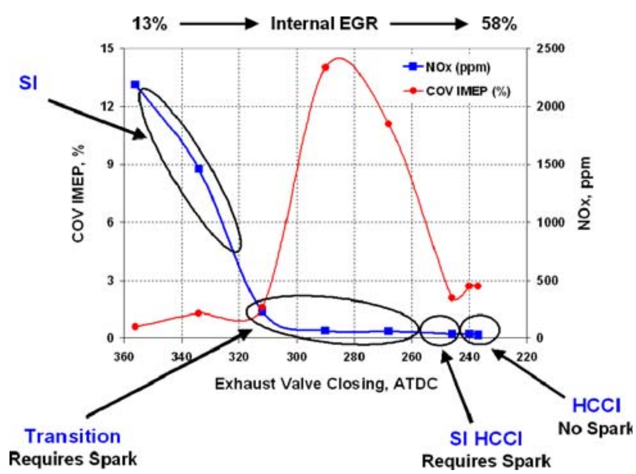
- Using fuel changes, SNL demonstrated a high-efficiency (>44% indicated efficiency), 2010-emissions-compliant (<0.2 g/hp-hr NOx, <0.05 filter smoke number) combustion strategy where ignition timing is simply controlled by injection timing, and peak pressure-rise rates are lower than for conventional diesel combustion.
- SNL completed a quantitative database showing the effect of EGR on soot in reacting diesel fuel jets. Results show that soot volume fraction decreases with decreasing ambient oxygen concentration, but the total soot in the jet cross-section increases and then decreases to zero as the ambient oxygen concentration decreases from 21% to 8%. The trend is caused by competition between soot formation rates and increasing residence time for soot formation.

- Oak Ridge National Laboratory (ORNL) demonstrated high-efficiency clean combustion (HECC) operation for an extended range of speed-load conditions in a multicylinder engine. They also investigated the transition from conventional to HECC operation and navigation through HECC space with no significant excursions in efficiency or emissions.
- SNL completed a unified modeling framework, completed preliminary staging studies, and initiated simulation of the optical hydrogen-fueled engine.
- Lawrence Livermore National Laboratory (LLNL) delivered a computationally efficient analysis procedure for detailed and accurate analysis of HCCI and premixed charged compression ignition (PCCI) combustion based on KIVA and multi-zone CHEMKIN (KIVA3V-MZ), validated it, and parallelized the code for even better computational efficiency.



Laser Image taken by SNL showing the presence of Hydroxyl Radical (Green) and Soot (Red)

- ANL achieved successful installation of their endoscope system into a Mercedes 1.7 liter CIDI engine and operated the engine under full-speed and full-load conditions while obtaining endoscope images
- SNL showed that the main .non-uniformities in HCCI combustion are due to thermal stratification resulting from heat transfer, and that these non-uniformities slow the heat release rate by sequential autoignition of progressively cooler regions.
- SNL developed and tested an emissions prediction method for predicting hydrocarbon (HC), carbon monoxide (CO), and carbon dioxide (CO_2) emissions during low-load stratified operation based on laser-induced fluorescence images of in-cylinder equivalence ratio.
- The University of Wisconsin Consortium identified HCCI combustion regimes in heavy- and light-duty engines using both low-pressure and high-pressure fuel injection and multiple injection strategies. They also showed that HCCI engine operating limits can be extended by operation with stratified combustion.



ORNL Research Showing Stability and NOx Emissions during the Transition from SI to HCCI Combustion Using Internal EGR

- The University of Michigan Consortium experimentally demonstrated potential HCCI engine control methods using variable valve events and identified characteristic times of in-cylinder effects for ~10 cycles. They also found a strong effect of wall temperature on combustion phasing with characteristic time of ~100 cycles.
- ORNL identified and characterized the existence of deterministic structure in the transition region between spark ignition and HCCI combustion modes.
- Los Alamos National Laboratory (LANL) continued development of the KIVA-4 code, including supplementing it with a grid-generation procedure to create the moving complex 3D grids found in

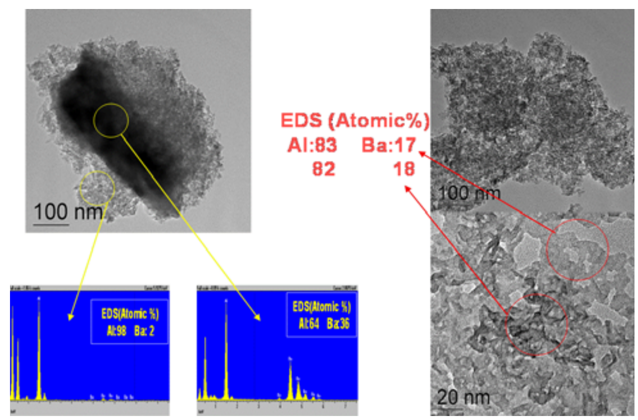
engines. In addition, they created a parallel version of KIVA-4 which allows KIVA-4 to run on multiple processors simultaneously.

- LLNL completed chemical kinetics models of combustion for two major fuel components, toluene and methyl cyclohexane, and for an oxygenated diesel fuel additive, dimethyl carbonate.
- ANL obtained OH* chemiluminescence images from hydrogen combustion using ultraviolet (UV) imaging that illustrate how hydrogen combustion proceeds under various fuel preparation conditions and stoichiometries. A correlation between heat release and OH* intensity was obtained.
- SNL conducted experiments using OH chemiluminescence to assess the effects of fuel injection variables on hydrogen engine operation and mixture formation.

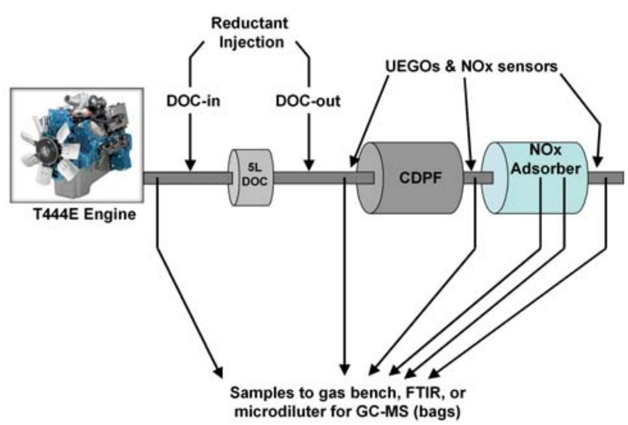
B. Energy-Efficient Emission Controls

The following project highlights summarize the advancements made in emission control technologies to both reduce emissions and reduce the energy needed for their operation.

- Pacific Northwest National Laboratory (PNNL) identified two morphological 'forms' of the storage Ba-phase in lean NOx trap catalysts – a 'monolayer' phase and a 'bulk' phase.
- PNNL detailed in-situ x-ray diffraction studies coupled with performance measurements showed that thermal deactivation can be most directly correlated with Pt particle size growth and can also be used to explain dramatic differences in the behavior of 'Simple Model' and 'Enhanced Model' lean NOx trap materials.
- PNNL developed a novel regenerable SOx adsorber. The composition is based on a non-precious metal on an inert silica support. It is capable of operation under the lean-rich cycling required for NOx traps with at least 90% SOx removal over the temperature range 250-550°C.
- ORNL continued lean NOx trap studies with in-situ measurements. Results have been published on reductant utilization, nitrogen selectivity, desulfation, temperature effects, and LTC-based regeneration.
- ORNL evaluated iso-octane, toluene, and 1-pentene reductants to confirm rank order of various hydrocarbon families in lean NOx trap regeneration.



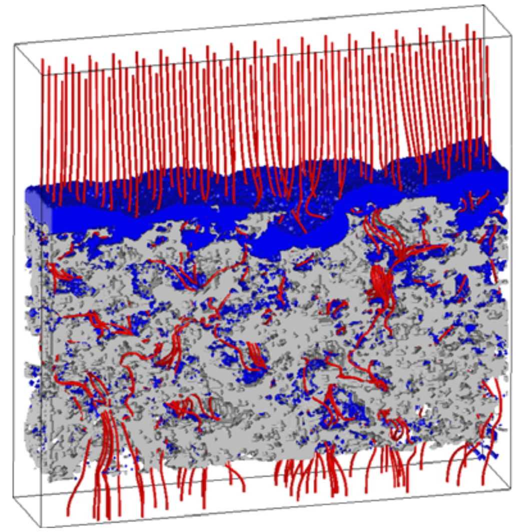
Transmission Electron Microscopy of Adsorber Catalyst Taken by PNNL



ORNL Test Set-Up to Study Hydrocarbon Reductant Regeneration of a NOx Adsorber Catalyst

- Ford Motor Company achieved Tier 2 Bin 5 emissions levels at low mileage using a urea-based selective catalytic reduction system with a mid-size diesel engine on a 6,000 lb gross vehicle weight rating (GVWR) light-duty truck. Tailpipe emissions levels were at 0.041 g/mi NOx and 0.001 g/mi PM.
- Several new catalyst formulations identified by SNL showed enhanced NOx conversion performance compared to the commercial ZNX catalyst material.

- ORNL developed a new reactor for Diffuse Reflectance Infrared Fourier-Transform Spectroscopy (DRIFTS) measurements along the length of catalyst washcoats.
- ORNL applied spatially resolved capillary inlet mass spectrometer (SpaciMS) and phosphor thermography (PhosT) instruments for quantitative and minimally invasive in-operando intra-catalyst measurement of transient species and temperature distributions, respectively.
- ORNL modified lean NOx trap regeneration strategies to generate engine-out hydrogen and other reformate products under net-lean conditions.
- Dimethyl ether (DME) was demonstrated by PNNL to be an excellent reducing agent for lean NOx traps, and mechanistic studies were initiated to determine why DME is an effective reagent and to determine effects of syngas on lean NOx trap performance.
- ORNL demonstrated greater than 90% NOx conversion for a hydrogen engine lean NOx trap system between 300 and 400°C, with an approximate fuel penalty less than 5%.
- ORNL supported the Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS) activity, which included administrative support, joint development of benchmark kinetics, and micro-scale catalyst modeling.
- PNNL created digital pore geometry maps for the Corning EX-80 cordierite substrate and developed a micro-scale discrete particle deposition model using the lattice-Boltzmann method.



Graphic Depiction of Soot Deposits and Streamlines in a Diesel Particulate Filter Model created by PNNL

- Caterpillar performed hot shake testing of straight-channel low-cost metal substrate deNOx catalyst prototypes that showed little difference in performance compared to current materials.

<u>C. Enabling Technologies</u>

Sensors, new instrumentation, and advanced catalyst designs are enabling technologies for achieving more efficient engines with very low emissions. The following highlights show the progress made during FY 2005.

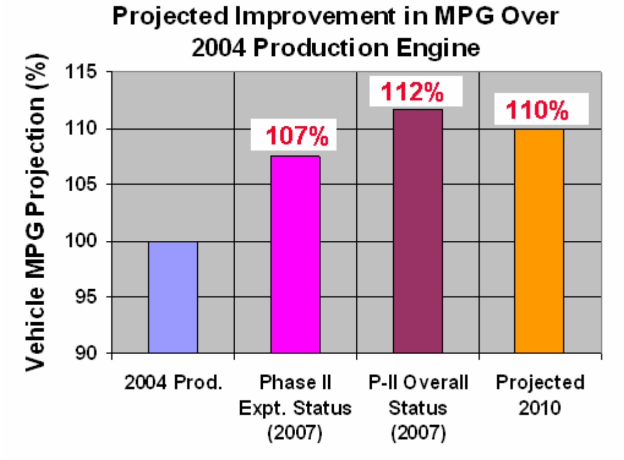
- Delphi demonstrated functional performance of their NOx sensor with over 10,000 vehicle miles accumulated, and subjected it to hot vibration and shock testing equivalent to 200,000 miles of vehicle operation (which it successfully passed).
- CeramPhysics successfully manufactured capacitor-type NOx and O_2 sensor bodies with a matrix of porous Rh-based electrodes varying in composition from 10/90 to 100/0 Rh/Pt ratio.
- The Envera variable compression ratio (VCR) mechanism was successfully packaged into an in-line 4-cylinder CIDI engine, demonstrating the manufacturing feasibility of VCR variants of production engines.

Heavy Truck Engine

With the advent of stringent emission standards, it is necessary to design engines as systems to achieve both high efficiency and low emissions. The following project highlights describe the progress made for both light- and heavy-duty engines during FY 2005.

- Cummins demonstrated 2010 emissions performance from a base engine architecture assuming a NOx reduction aftertreatment system.

- Caterpillar validated a diesel engine system capable of 45% thermal efficiency while meeting 2007 on-highway heavy-duty engine emissions and a diesel engine system capable of 50% thermal efficiency while meeting 2010 on-highway heavy-duty engine emissions levels using simulation.
- Detroit Diesel Corporation (DDC) demonstrated brake thermal efficiency of 44% at 2007 emissions levels on the multi-cylinder engine test-bed and developed an advanced combustion and engine subsystem roadmap to meet post 2007 EPA-stipulated emissions levels, including 2010 regulations and beyond.

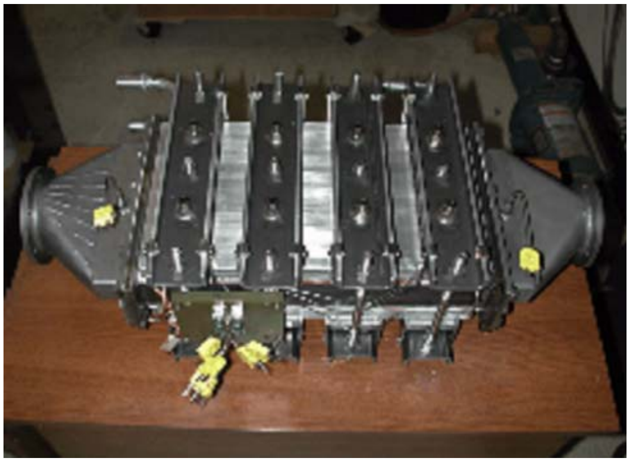


DDC Projections of Project Heavy-Duty Vehicle Efficiency Improvements

Waste Heat Recovery

Several technologies are being pursued to capture waste heat from advanced combustion engines, including electricity generation from turbochargers, thermoelectrics, and others. Following are highlights of the development of these technologies during FY 2005.

- Caterpillar completed testing of their electric turbocompound system (electricity generation from turbocharger) and predicted 3 to 5 percent improvement in fuel consumption from using the system.
- General Motors quantified the effect of reduced alternator load and increased vehicle weight on the fuel economy of representative vehicles, and evaluated suggestions for possible methods of achieving fuel economy gains using thermoelectric (TE) technology. They also achieved ~2 W output power for superlattice-based TE devices and 13% energy conversion efficiency for superlattice/bulk segmented/cascaded TE devices.
- BSST conceived and modeled a system architecture using AVL's ADVISOR model.
- United Technologies Research Center designed a first-generation thermoelectric generator (TEG) and measured its performance. Process aflow sheets were created to project manufacturing and selling costs, and market acceptance criteria were determined and compared to deduce selling price at the system level.
- The University of Michigan completed a detailed WAVE analysis of the 6-cylinder Cummins ISX engine showing that a one TEG per cylinder configuration permits an energy extraction level which is 90% greater per cylinder compared to the three-into-one design.
- Hi-Z Technology, Inc. achieved >530,000 equivalent miles in road tests of its 1 kW diesel truck thermoelectric generator and achieved successful laboratory and test cell tests on a 300 Watt automobile exhaust thermoelectric generator.



Hi-Z 300 Watt ThermoElectric Generator to be Mounted on a Heavy-Duty Vehicle for Testing

Off-Highway Engine Efficiency R&D

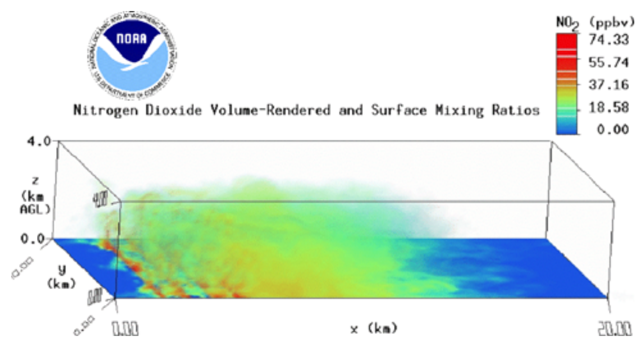
Off-highway vehicles are coming under more stringent emission controls similar to those for highway vehicles. However, their typical duty cycles place unique demands on emission control systems. Following are highlights of off-highway vehicle emission control development during FY 2005.

- Cummins identified a number of emissions architectures for meeting the Tier 4 Interim emissions requirements and conducted combustion computational fluid dynamics and cycle simulation analysis to recommend combustion and air handling hardware for experimental validation.
- GE Global Research compared engine performance with “fast” and “slow” needle lift response and quantified the impact of response on fuel consumption and emissions. GE also performed optimization studies with the latest generation high-pressure common rail system.
- John Deere optimized its low pressure loop EGR system and achieved the goal of less than 2 g/kWh NOx and less than 0.02 g/kWh PM over the ISO 8178 eight-mode test.
- ORNL demonstrated that applying higher fuel rail pressure, in combination with ultra-low sulfur diesel fuel and urea-SCR NOx control technology, is a high-potential candidate for achieving the interim Tier 4 off-road heavy-duty engine emission standards.

Health Impacts

The Health Impacts activity has been studying the hazards to human health posed by vehicle emissions. Following are highlights of the work conducted in FY 2005.

- ORNL completed a study for the Knox County Municipal Planning Organization on ambient air quality in truck travel centers; incorporated a shorter wavelength laser into remote PM measurement instrument for better resolution of small particles; and demonstrated high sensitivity of ultraviolet method for remote NOx measurement.
- NREL completed analysis of 1998-2002 or 2003 ambient ozone precursor and ozone data from many U.S. monitoring locations.
- Lovelace Respiratory Research Institute discovered that emissions from malfunctioning gasoline-, diesel-, and compressed natural gas (CNG)-fueled vehicles (high emitters) were up to 5 times more toxic to the lung per unit of mass than normal emissions, and that crankcase oil emissions can be more toxic to the lung than fuel combustion emissions and are a primary cause of higher toxicity per unit of mass of emissions from high emitters.



ORNL Simulation of NO_2 Flux into the Atmosphere from a Dual Line Source such as a Highway

Future Directions

Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

The focus in FY 2006 for combustion and related in-cylinder processes will be on advancing the fundamental understanding of combustion processes and improving the performance of these processes. To advance fundamental understanding of combustion processes, several projects will work to improve the relevance and accuracy of their measurement techniques and modeling tools.

Measurement techniques that will be improved or used more extensively include ANL's x-ray fuel spray measurements, SNL's optical diagnostics and analytical techniques for LTC multiple/early/late injection schemes, and ANL's endoscope system for acquiring images of LTC combustion regimes in a diesel engine. Modeling capabilities that will be improved, expanded, or validated include LLNL's KIVA3V-MZ-MPI and KIVA-4 codes, SNL's high-fidelity large eddy simulation calculations for an optical hydrogen-fueled engine and laser-induced fluorescence-based prediction method to estimate NOx emissions from stratified HCCI operation, the scavenging system of SNL's free-piston engine, ORNL's nonlinear analysis technique for characterizing HCCI and HCCI-like combustion modes and physics-based spark ignition HCCI engine model for evaluating control strategies, and LLNL's combustion model for examining fuel components and mixtures. Engine control experiments conducted by the University of Michigan Consortium will expand and refine our understanding of mode transitions and thermal transients in HCCI operation.

In addition to working on measurement and modeling tools, several parametric studies will be conducted/continued to improve the performance of combustion processes. SNL will evaluate the effect of engine boost on low-temperature combustion systems and on the fuel conversion efficiency loss typically observed with high dilution levels; determine the extent to which high-efficiency clean combustion can be achieved with more traditional fuels such as diesel fuel, biodiesel, and Fischer-Tropsch paraffins; determine how combustion of pre-main-injection fuel affects combustion and soot formation of a second main-injection and investigate the effect of intake air pressure boost and EGR cooling on soot formation at high-EGR, LTC conditions; and investigate the importance of boundary-layer combustion in slowing the heat release rate during HCCI combustion. ORNL will identify and characterize injection strategies and injector characteristics (e.g., orifice diameter, number of holes, etc.) for expanding the speed/load operating range of HECC and improving transitions between normal and HECC modes as well as within HECC modes.

Six new high-efficiency clean combustion projects will continue into 2006. Cummins will develop state-of-the-art diesel combustion technology into commercially viable light- and heavy-duty engines which are capable of providing significantly improved thermal efficiency while achieving ultra-low NOx and particulate emissions. GM Powertrain and Sturman Industries will work together to develop high-efficiency clean combustion engine hardware for spark ignition and compression ignition ICEs. Caterpillar will identify and/or advance the required technologies to enable a low-temperature, high-efficiency combustion solution for commercial 2010 on-highway truck or 2014 non-road machine applications. International Truck and Engine will develop a production-capable diesel engine using HCCI combustion capable of achieving the 2010 EPA heavy-duty engine emissions standards at conventional power density with improved fuel consumption and emissions control technology compatibility. John Deere Product Engineering Center will prove the concept of cooled EGR, a diesel particulate filter, and a three-way catalyst to meet off-road emission standards. Mack Trucks, Inc., will attempt to improve the fuel economy by 15% while meeting 2010 emissions regulations through a combination of advanced engine technology and air-powered hybridization called an air power assist (APA) engine. The concept employs the engine as a compressor to store energy as compressed air during braking, and makes that energy available to power the engine during vehicle acceleration. The key technology required for the APA engine concept is a fully-flexible engine valve actuation system.

In addition to the six projects above, five new university research projects will contribute to furthering the understanding of advanced combustion regimes. A university consortium led by the University of Michigan will determine the practical boundaries of low-temperature combustion engines and develop methods to extend those boundaries. The University of Wisconsin will develop methods to control pollutant emissions in-cylinder in LTC diesel engines. West Virginia University Research Corporation will study and develop practical means by which thermochemical recuperation can be integrated with LTC. Texas A&M will initiate a project to apply both the first and second laws of thermodynamics to develop improved engine design concepts by reducing irreversibilities, thereby increasing efficiency. A new project at Michigan State University will investigate their proposed engine concept employing a high-compression-ratio, modified Atkinson combustion cycle that uses a novel low-pressure, direct-injection fuel system and electronic-pneumatic valve actuation.

Work will continue at ANL and SNL to investigate hydrogen engine combustion using OH chemiluminescence imaging. Using direct injection, hydrogen engines have the potential to be as efficient at advanced CIDI engines.

B. Energy-Efficient Emission Controls

Technologies under consideration for reducing NOx emissions include NOx adsorbers, lean NOx catalysts, and selective catalytic reduction (SCR). In addition, work in the energy-efficient emission controls activity in FY 2006 will include developing PM reduction technologies, desulfurization strategies for improving the durability of emission control technologies, and models and analytical techniques to facilitate better understanding and optimization of emission control technologies.

A considerable amount of work on NOx adsorbers is planned for FY 2006. ORNL will continue to develop and apply diagnostics to optimize engine-catalyst system-level parameters to enhance diesel efficiency and viability, and quantify select effects of catalyst deactivation mechanisms on the efficiency of NOx reduction reactions. ORNL will also quantify DRIFTS spectra for K-based catalysts, expand the temperature range of measurement (200 and 500°C), further characterize catalysts with respect to sulfation, and implement the in-situ DRIFTS reactor for washcoated samples. In addition to these research projects, ORNL will continue to support the CLEERS activity, including administrative support, joint development of benchmark kinetics, and micro-scale catalyst modeling.

Two PNNL projects also have plans to study NOx adsorbers in 2006. These projects will continue BaO morphology studies; perform detailed characterization of alternative materials; study the Pt particle size dependence of the NO oxidation reaction; study CLEERS Umicore samples; and further refine function-specific measures of lean NOx trap ‘aging’. A new project is being initiated at the University of Houston to conduct kinetic and performance studies of the regeneration phase of model Pt/Rh/Ba NOx adsorbers for design and optimization, and another new project at the University of Kentucky will investigate aging mechanisms in lean NOx traps. Finally, ORNL will investigate the potential for improved NOx conversion of lean NOx trap regeneration while targeting minimal fuel penalty, and improve the understanding of desulfation phenomena through engine-based rapid sulfation/desulfation experiments.

In 2006, PNNL will complete mechanistic work in 2006 to determine why DME is such a good reductant over lean NOx catalysts and will examine DME/methanol blends as reductants. ORNL will evaluate commercial HC-SCR catalysts (Pt, Cu, and Ag) and PNNL HC-SCR catalysts under a variety of engine conditions. ORNL will also continue evaluating hydrogen engine NOx emissions reduction technologies, including NOx adsorbers, SCR catalysts, and lean NOx catalysts, with a core reactor to more accurately assess fuel penalty constraints.

Other projects concerned with PM emission reduction are being conducted at PNNL and Caterpillar. PNNL will incorporate more sophisticated soot oxidation mechanisms into their pore-scale models, including heat transfer, surface catalytic reactions, and transport of active gaseous species, and will perform further parametric studies to characterize the effects of microstructural substrate features. Caterpillar will complete engine testing and modeling of full-scale straight-channel low-cost metal substrate deNOx catalyst prototypes with a new design to verify improved emissions performance.

Ford Motor Company will complete evaluation of their 120,000-mile aged emission control system test and continue development of improved catalyst formulations, NOx sensors, and ammonia sensors.

C. Enabling Technologies

In 2006, Delphi will test its NOx sensor with the new Gen II controller, and CeramPhysics will continue characterizations and long-term testing of their NOx sensor body, finish development of electronic control of partial oxygen pressure inside the assembled sensor and its temperature, and incorporate NOx and O_2 sensor bodies into fully assembled NOx sensors. Honeywell International will initiate a new project to implement fast-response PM and NOx sensors to control a low-pressure EGR system and implement particle trap operational diagnostics to enhance fuel use efficiency and reduce emissions.

In addition to sensor work, two new projects will focus in 2006 on actuation to facilitate advanced LTC processes. Delphi Automotive Systems, LLC will develop and demonstrate an optimal, cost-effective systems approach to diesel engine variable valve actuation to enable an expanded operating range of HCCI and regulation of the temperature of aftertreatment catalysts. Envera LLC will develop a fast-response actuator for adjusting compression ratio in variable compression ratio engines and demonstrate it through testing and computer modeling. Variable compression ratio has the ability to attain 30 percent improvement in fuel economy concurrent with an increase in vehicle performance, at significantly lower production cost than hybrid electric vehicle technology.

Heavy Truck Engine

Several advanced engine design activities will be completed in 2006 with the goal to demonstrate 50% brake thermal efficiency while meeting 2010 emissions standards. Cummins will use the information developed in 2005 about advanced combustion (cooled EGR combined with high-pressure multiple fuel injection), waste heat recovery (an organic Rankine cycle device that produces electricity to offset engine auxiliary loads), and exhaust emission treatment (devices to reduce NOx and PM emissions) to prepare a truck using these technologies for demonstration. Caterpillar will further develop and refine the fuel economy building blocks identified in 2005 (reduced friction piston rings, high-efficiency series turbochargers, cylinder head with improved port flow and increased peak cylinder pressure capability, compact high-efficiency cooling system, high-pressure injection system, and variable intake valve actuation) along with efficient NOx aftertreatment technology to enable a demonstration of a 50% overall thermally efficient engine capable of meeting 2010 emissions standards. DDC will solidify and systematically evaluate the components of the advanced technology roadmap they developed in 2005 with the objective of completing a model-based controls algorithm for combining advanced combustion modes (homogeneous charge compression ignition and other low-temperature concepts) to improve the NOx-BSFC trade-off at low NOx levels such that degradation of BSFC is significantly reduced, along with exhaust aftertreatment system (urea-SCR catalyst and a diesel particulate filter) control to produce integrated engine and emission control systems that are robust and enhance seamless transition between operating modes.

Waste Heat Recovery

Research will continue in FY 2006 on turbochargers, thermoelectrics, and other technologies for capturing and utilizing waste heat from advanced combustion engines, and four new projects will be initiated in this important area.

Five projects will continue using thermoelectrics to extract useful energy from exhaust and cooling water heat. General Motors will evaluate the thermoelectric properties of type I clathrates, solid solution-based skutterudites, and nano-structured bulk materials; optimize superlattice-based thermoelectric devices; develop bulk material-based thermoelectric devices; and conduct an economic feasibility study of automotive thermoelectric waste heat recovery technology. BSST will test subsystem equipment over typical drive conditions, and models will be updated and validated. These results will be used to update the overall system performance model, yielding a new set of performance predictions based on the test results of subsystem equipment operating in a laboratory environment. United Technologies Research Center will conduct base technology qualification and verification at the material level, proof-of-concept experiments using cathodic arc as a deposition process as well as non-deposition processes for heterogeneous nanocomposites, and method development for the enhancement of techniques that are used to measure thermoelectric performance and conversion efficiency at the material and module level. The University of Michigan will model a full 6-

cylinder Cummins ISX engine with integrated TEG units and include the turbocharger and exhaust gas recirculation (EGR) bypass systems as sources of heat. Hi-Z Technology, Inc. will test 2 W and 20 W modules as building blocks for larger quantum well (QW) modules and will improve high-temperature limits and reduce parasitic losses for QW film to approach the predicted 25% efficiency level.

Additionally there are four new projects that will each target fuel efficiency improvement of 10% or more through waste heat recovery. Caterpillar's Technology and Solutions Division will initiate development of a new air management and exhaust energy recovery system, which is likely to include electric turbocompounding and high-efficiency air system technology. John Deere Product Engineering Center will develop an electrically coupled exhaust energy recovery system using a series power turbine approach, targeting a 20% increase in net engine power output in addition to 10% improvement in fuel economy. Cummins will apply existing technology to modify and replace current heat transfer components to achieve an efficient waste heat recovery system. Mack Powertrain Division of Volvo Powertrain Corporation will focus on a high-fuel-economy, heavy-duty, constant-speed truck engine, optimized via unique energy recovery turbines and facilitated by a high-efficiency continuously variable powertrain.

Off-Highway Vehicle Emission Control R&D

Progress will continue in FY 2006 on development of off-highway vehicle emission control technologies. Cummins will complete analysis and experimental work leading to the selection of the prime path Tier 4 Interim emission architecture for further optimization. GE Global Research will complete performance of other hardware modifications to the common rail system, possibly including nozzle, orifice plate and injector accumulator volume changes. John Deere will complete their final report, and Michigan Technological University will use the data collected to model the new aftertreatment technology. In their CRADA with Deere, ORNL will evaluate the influence of alternative fuels on engine efficiency, on the performance of urea-SCR systems, and on PM formation under conditions of high rail pressure.

Health Impacts

A variety of health impact studies will support the Advanced Combustion Engine Sub-Program’s goals in FY 2006. ORNL will continue deployment of the remote sensing instrumentation; link field measurements to air quality models and health impacts; and apply higher time resolution measurements of air toxics in order to understand mobile source impacts. NREL will begin a proximate ozone modeling study in the southeast Michigan region in collaboration with state and local government groups and industry representatives in that area. Lovelace Respiratory Research Institute will complete work to confirm or refute health importance of nanoparticle (<50 nm) components of diesel emissions, as well as relative importance of black carbon- vs. non-solid condensate-based particles, and will determine causal components responsible for unanticipated toxicity associated with emerging power technologies. In a new project, the Health Effects Institute will determine before widespread commercial deployment whether or not the new heavy-duty diesel engines (2007 and 2010 EPA emissions standards compliant) may generate anticipated toxic emissions which could adversely affect the environment and human health.

Honors and Special Recognitions

- Paul Miles (SNL) Invited Paper and Keynote Lecture to the Fifth Symposium Towards Clean Diesel Engines, June 2005.
- The paper “The Influence of Charge Dilution and Injection Timing on Low-Temperature Diesel Combustion and Emissions,” (SAE Paper No. 2005-01-3837) by Kook S, Bae C, Miles PC, Choi D, and Pickett LM (SNL) was selected for inclusion in 2005 SAE Transactions.
- Charles Mueller (SNL) received the Society of Automotive Engineers Arch T. Colwell Merit Award, for his paper entitled "Effects of Oxygenates on Soot Processes in DI Diesel Engines: Experiments and

Numerical Simulations," SAE Technical Paper 2003-01-1791. This was one of 11 papers honored in 2004 for being most innovative and original out of approximately 2,500 papers published during the preceding year.

- Charles Mueller (SNL) received the Society of Automotive Engineers Lloyd L. Withrow Distinguished Speaker Award. This was one of 8 such awards presented in 2005 to recognize individuals who have received SAE's Oral Presentation Award more than twice.
- Joseph C. Oefelein (SNL) invited paper: "Large Eddy Simulation for Turbulent Combustion and Propulsion," Progress in Aerospace Sciences, June 2005.
- Joseph C. Oefelein (SNL) invited paper: "Mixing and Combustion of Cryogenic LOX-H2 Shear-Coaxial Jet Flames at Supercritical Pressure," Combustion Science and Technology, May 2005.
- Joseph C. Oefelein, R. W. Schefer and R. S. Barlow (SNL) invited paper: "Toward Validation of LES for Turbulent Combustion," AIAA J, May 2005.
- Joseph C. Oefelein (SNL) invited paper: "Large Eddy Simulation of Liquid Rocket Injection and Combustion Processes," Proceedings of the Computational and Engineering Science Conference, Washington DC, April 26-27, 2005.
- Salvador M. Aceves (LLNL) was invited to deliver a seminar at the SAE 2005 seminar on HCCI, September 2005, Lund, Sweden.
- John Dec (SNL) was invited to be the keynote speaker for the 2004 SAE Fall Powertrain and Fluid Systems Conference, Tampa, FL, October 2004.
- John Dec (SNL) was an invited speaker at the SAE Homogeneous Charge Compression Ignition Symposium, Lund, Sweden, September 2005.
- Richard Steeper of SNL served as Co-Vice-Chair of Combustion for SAE's Fuels and Lubricants Activity in 2005.
- Brian West (ORNL) received the Society of Automotive Engineers Excellence In Oral Presentation award for presentation of "Time-resolved Laser-Induced Incandescence Measurements of Particulate Emissions During Enrichment for Diesel Lean-NOx Trap (LNT) Regeneration" at the SAE 2005 World Congress (April 2005).
- Chuck Peden (PNNL) gave an invited presentation, "Fundamental Studies of Catalytic NOx Vehicle Emission Control," at the University of Pennsylvania, Philadelphia, PA, October 2004.
- Chuck Peden (PNNL) gave an invited presentation at the 2005 Meeting of the Pacific Coast Catalysis Society, Berkeley, CA, March 2005.
- Janos Szanyi (PNNL) gave an invited presentation at the American Chemical Society National Meeting, San Diego, CA, March 2005.
- ORNL staff member James E. Parks II delivered a keynote presentation at the 19th North American Catalysis Society Meeting in Philadelpia, held May 22-27, 2005.
- The paper "Modeling the Effects of EGR and Injection Pressure on Soot Formation in a High-Speed Direct-Injection (HSDI) Diesel Engine Using a Multi-Step Phenomenological Soot Model," (SAE Paper No. 2005-01-0121) by Tao F, Liu Y, RempelEwert BH, Foster DE, Reitz RD, Choi D (University of Wisconsin) and Miles PC (SNL) was selected for inclusion in 2005 SAE Transactions.
- The presentation "A Mechanistic Model for Particle Deposition in Diesel Particulate Filters Using the Lattice-Boltzmann Technique," by M. Stewart, D. Rector, G. Muntean, and G. Maupin (PNNL), received the Best Presentation award from the 2004 American Ceramic Society Cocoa Beach Meeting.
- Jihui Yang (General Motors) was elected to the board of directors of the International Thermoelectric Society, June 2005.
- The GE Global Research off-highway engine efficiency R&D project won the GE Rail Technology Leadership for Innovation Award – January 2005.

Invention and Patent Disclosures

- Controlling and Operating Homogeneous Charge Compression Ignition (HCCI) Engines, Daniel L. Flowers, United States Patent 6,923,167, August 2, 2005.
- Filed U.S. patent application #11/095,256, “Fuel Mixture Stratification as a Method for Improving Homogeneous Charge Compression Ignition Engine Operation.” (John Dec, SNL)
- Reitz, R.D., Rutland, C.J., Jhavar, R., “Engine Valve Actuation for Combustion Enhancement,” U.S. Patent 6,736,106, May 2004.
- Method of Generating Hydrocarbon Reagents from Diesel, Natural Gas and other Logistical Fuels, patent filed May 2005 (PNNL).
- Catalyst System and Method for the Reduction of NOx, patent filed Dec. 2004 (PNNL).
- Catalyst System and Method for the Reduction of NOx with SOx, patent filed Dec. 2004 (PNNL).
- An international patent (WO 2005/077498 A1) titled “Sulfur Oxide Adsorbents and Emissions Control” was awarded to David King and LI Liyu of PNNL on August 25, 2005.
- Ron Graves, Brian West, Shean Huff, James Parks, "Advanced Engine Management for Control of Exhaust Species," Invention Disclosure filed September 2005.

The remainder of this report highlights progress achieved during FY 2005 under the Advanced Combustion Engine R&D Sub-Program. The following 56 abstracts of industry, university, and national laboratory projects provide an overview of the exciting work being conducted to tackle tough technical challenges associated with R&D of higher efficiency, advanced internal combustion engines for light-duty, medium-duty, and heavy-duty vehicles. We are encouraged by the technical progress realized under this dynamic Sub-Program in FY 2005, but we also remain cognizant of the significant technical hurdles that lie ahead, especially those to further improve efficiency while meeting the EPA Tier 2 emission standards and the heavy-duty 2010 engine standards. In FY 2005, we implemented 21 new competitively-selected projects that broaden the working relationship with our industrial and university partners to overcome additional barriers that hinder the widespread availability of high-efficiency, clean, advanced internal combustion engines.

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